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ORIGINAL RESEARCH PAPER

Enhancing the Monsanto Process via Lithium Iodide Addition

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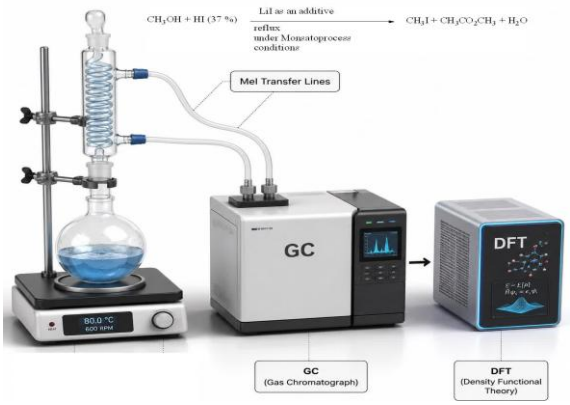
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A B S T R A C T

The Monsanto process is one of the most important industrial routes for acetic acid production, in which methyl iodide (CH_3I) serves as a key intermediate. In this study, lithium iodide (LiI) was investigated as a promoter for the conversion of methanol to methyl iodide under conditions analogous to those of the Monsanto process. The objective was to evaluate the effects of temperature, hydrogen iodide (HI) solution volume, LiI loading, and reaction time on the formation of CH_3I and on the overall composition of the reaction mixture. The HI solution used in the experiments contained 37% HI, 30% acetic acid, and 33% water under reflux conditions. Product distributions were monitored by gas chromatography at 2 h intervals over 6 h. The experimental results showed that temperature had a significant effect on methyl iodide formation, with 100 °C being identified as the optimum reaction temperature. The highest CH_3I concentration was obtained using 20 mL of HI, 20 mL of methanol, and 1.00 g LiI, giving 8.8% after 2 h and 9.1% after 6 h. Increasing the HI volume to 30 mL significantly reduced the CH_3I concentration to 1.6–2.2%, while using 2.00 g LiI gave 7.1–8.7% CH_3I. In the absence of LiI, CH_3I increased from 6.5% to 7.3%. A theoretical study based on density functional theory (DFT) conducted to examine the interactions of methanol with H^+, Li^+, HI, and LiI. The combined experimental and theoretical results indicate that LiI promotes methyl iodide formation and may improve the efficiency of Monsanto-process-related chemistry.



1. Introduction

Acetic acid is a chemical compound widely used in both laboratories and industrial processes. It is a key precursor in the synthesis of vinyl acetate monomer (VAM), acetic anhydride, and various solvents [1-4]. Furthermore, its antimicrobial properties enable its use in treating ear infections. Additionally, its application as a natural herbicide provides an effective method for weed control in organic farming. Numerous catalysts for acetic acid synthesis have been reported, such as rhodium (III) iodide (RhI_3),tris (triphenylphosphine) rhodium iodide ($(Ph_3P)_3PRhI$), tris (triethylphosphine) rhodium iodide ($(Et_3P)_3PRhI$), and iridium (III) iodide (IrI_3) (Figure 1) [5-9]. Lithium iodide (LiI) is utilized in various industrial processes, such as the reduction of CO_2 to C2+ products [10-13].

In acetic acid synthesis, it has been reported that the addition of LiI enhances the reaction during the carbonylation of methanol with CO_2 and H_2 over Ru-based catalysts [14]. Furthermore, LiI improves the efficiency of the Rh catalyst in the Monsanto process by stabilizing the $[Rh(CO)_2I_2]^-$complex and increasing the reaction rate [14, 15]. A mechanism has been reported in which the addition of LiI increases the rate of the Monsanto process by accelerating the conversion of methanol to methyl iodide via a bimolecular nucleophilic substitution (S_N2) reaction. The advantages of utilizing LiI in the carbonylation of methanol for acetic acid synthesis include: 1. the high solubility of the

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reagent in methanol; 2. a reduction in the required reaction temperature; 3. minimization of by-products formation [16]. Therefore, in this study, the synthesis of methyl iodide from methanol using LiI as a promoter was investigated under various conditions.

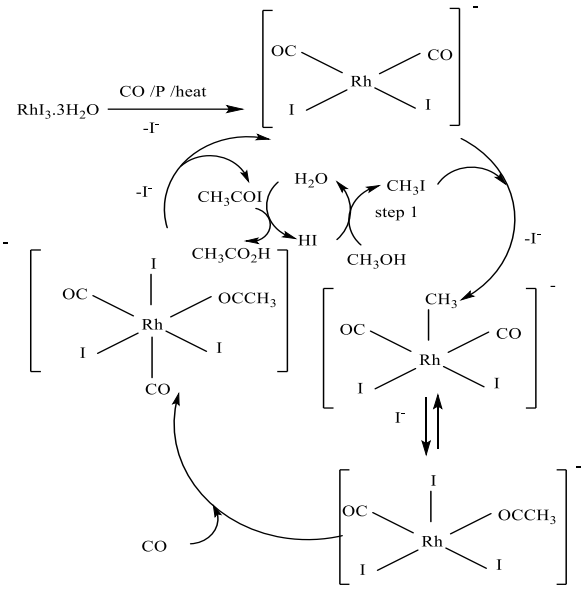


Figure 1. Acetic acid synthesis process

Source: Research Findings

1.1. Density functional theory calculation

Density Functional Theory (DFT) is a modern computational method used in quantum chemistry and physics. It is a theoretical approach widely employed to study the geometric and electronic structure of compounds, as well as thermodynamic properties and kinetics parameters involved in chemical and physical reactions [4, 17-21]. DFT addresses these problems by focusing on the electron density ρ(r) rather than dealing with the complex many-electron wavefunction $\Psi(r_1, r_2,\ldots,r_N)$. This approach is based on the Hohenberg–Kohn theorems. This theory uniquely determines the ground-state (GS) wavefunction and energy of a system, and the GS can be obtained by minimizing a functional E[ρ] over all possible densities. [22]

So, in this study, the DFT method was used Gaussian 09 (G09) at the B3LYP/6-31G level of theory to investigate the role of LiI as a promoter in the Monsanto process. The enthalpy change for reactions (5-8) was calculated in the gas phase. The results show that the interaction between methanol and Li^+ and LiI is more negative than the interaction of CH_3OH with H^+ and HI. These results confirm the experimental data reporting that LiI as promoter, increases the rate of acetic acid production. Furthermore, to investigate the role of LiI as a promoter in the Monsanto process, the electronic parameters of these interactions were examined (Table 5). According to the data reported in Table 4 ($\Delta E = E_{LE^+} - E_{H\,Nu}$), electron transfer from methanol to Li^+ and LiI was more favorable than electron transfer to H^+ and HI.

5. $CH_3OH\ (l) + H^+(aq) \longrightarrow CH_3OH_2^+(aq)$ $\triangle$ = -115.65 a.u

6. $CH_3OH\ (l) + Li^+(aq) \longrightarrow CH_3OHLi^+(aq)$ $\triangle$ = -123.01 a.u

7. $CH_3OH\ (l) + LiI\ (aq) \longrightarrow CH_3OHLi^+(aq)$ $\triangle$ = -134.71 a.u

8. $CH_3OH\ (l) + HI\ (aq) \longrightarrow CH_3OHHI^+(aq)$ $\triangle$ = -127.67 a.u

2. Method

2.1. Methodology

In this study, all chemicals were purchased from Sigma-Aldrich and used as received, without further purification. The progress of the reaction was monitored using via GC **(**using a CP-WAX52CB column equipped with a TCD detector).

2.2. Synthesis of HI used in this study under conditions similar to those of the Monsanto process

The synthesis of methyl iodide was performed under conditions analogous to the those of the Monsanto process. Specially, hydrogen iodide (HI) was prepared according to Reaction 1, followed by the addition of acetic acid. The resulting data are reported in Table 1.

1. $I_2(s) + CO(g) + H_2O(l) \xrightarrow[T=130\ ^oC]{P=5.5\ bar} HI(aq) + CO_2(g)$

RhI_3 as catalyst

Table 1. Composition (wt%) of compounds in the HI solution determined by titration and GC analysis.

compound	HI	CH3CO2H	H2O
percent	37	30	33

Source: Research Findings

2.3. General procedure for the synthesis of methyl iodide from methanol

Various volumes of 37% HI solution, methanol, and specified amounts of LiI were introduced into a reaction vessel equipped with a reflux condenser (Figure 2). The reaction was performed under various conditions, and the reaction progress was monitored by GC at regular time intervals. In each experiment, methanol was added dropwise to minimize the formation of by-product (dimethyl ether and methyl acetate) (Reactions 2-4).

2. $CH_3OH \underset{heat}{\overset{HI\ and\ LiI}{\rightleftharpoons}} CH_3I + H_2O$

3. $CH_3OH + CH_3CO_2H \underset{heat}{\overset{HI\ and\ LiI}{\rightleftharpoons}} CH_3CO_2CH_3 + H_2O$ MeOAc

4. $CH_3CO_2CH_3 \underset{heat}{\overset{HI\ and\ LiI}{\rightleftharpoons}} CH_3CO_2H + CH_3I$



Figurer 2. Setup of synthesis of methyl iodide.

Source: Research Findings

2.3.1. Optimization of temperature for synthesis of methyl iodide

30 mL of 37% HI solution was added to a 100 mL flask equipped with a condenser, a separatory funnel, and a pump for circulating cold water. To reduce the formation of by-products such as methyl acetate (MeOAc) and dimethyl ether, 20 mL of methanol was added dropwise to the solution using a separatory funnel over 30 minutes at room temperature (Figure 2). The reaction progress was monitored by GC for 6 hours, and the samples were analyzed at 2-hour intervals. The data obtained at various temperatures are reported in Table 2.

2.3.2. Synthesis of methyl iodide under various conditions at 100 ◦ C

According to the data reported in Table 2, the optimal temperature is 100 °C. Consequently, various parameters were investigated to determine the optimal conditions for the conversion of methanol to methyl iodide. The experiments summarized in Table 3 were carried out using the procedure described above.

3. Results and Discussion

To investigate the effects of reaction temperature and time on the product distribution, the composition of the HI–methanol system was examined at room temperature, 50 °C, and 100 °C after reaction times of 2, 4, and 6 h, as shown in Table 2.

Table 2. Percentage of various compounds at different temperatures.

compound	HI	CH3I	MeOAc	MeOH	CH3CO2H	H2O
Run 1: the solution contained 30 mL of HI (37%) and 20 mL of absolute methanol at r.t.						
Percent at 2 h	28.1	3.5	16.5	17.2	3.1	31
Percent at 4 h	28.0	4.0	17.5	17.8	2.8	28.8
Percent at 6 h	26.0	4.5	17.0	17.0	2.4	33.0
Run 2: Same conditions as Run 1, but conducted at 50 ◦C.						
2 h	24.5	5.1	17.9	14.8	4.3	33.2
4h	23.7	6.0	17.2	14.3	4.2	33.5
6h	21.2	6.6	20.2	14.7	3.8	33.3

Run 3: Same conditions as Run 2, but conducted at 100 °C.						
2h	20.7	5.9	16.7	17.2	4.5	31.1
4h	20.55	6.0	17.0	16.4	4.3	31.8
6h	18.8	6.5	17.2	18.2	4.3	34.3

Source: Research Findings

The data reported in Table 2 show that is consumed the consumption of hydriodic acid increased with increasing temperature and reaction time increase; however, this results in only a modest decrease in its concentration from 28.1 % at 2 h to 26.0 % at 6 h. Increasing the temperature to 50 ºC accelerates this process, reducing the HI concentration to 21.2 % after 6 h. Finally, the most pronounced depletion occurs at 100 ºC, where the HI concentration reaches a minimum value of 18.8 % after at the 6 h, likely because the reaction proceeds via a bimolecular nucleophilic substitution (S_N2) mechanism. According the data reported in Table 2, the concentration of CH_3I increases moderately from 3.5 % to 4.5 % over 6 h at room temperature. However, at elevated temperatures of 50 °C and 100 °C, the CH_3I concentration increases to 6.6 % and 6.5 %, respectively after 6 h. While the concentration of methyl acetate remains relatively stable at room temperature (16.5 %-17.5 %), it reaches a maximum of 20.2 % at 50 ºC after 6 h. At 100 ºC, the MeOAc concentration stabilizes within a slightly lower range of 16.7 %-17.2 %. The concentration of acetic acid remained low throughout the process, ranging from 2.4 % to 4.5 %. This behavior can be attributed to competing esterification and hydrolysis side reactions in the strongly acidic aqueous medium, causing the system to approaches multicomponent thermodynamic equilibrium.

In addition, the concentration of water remained high and relatively stable throughout all experiments, fluctuating within a narrow range of 28.8 % to 34.3 %. The water content is primarily governed by the initial solvent composition and esterification pathways. The highest water concentration (34.3 %) was recorded at 100 ºC after 6 h. Likewise, the minor variations in methanol concentration, particularly its persistence at 100 ºC (18.2 % at 6 h), further suggest that the system reached a steady-state or equilibrium distribution under sealed conditions, with alcohol consumption balanced by possible regeneration pathways.

Table 3 presents an evaluation of the factors influencing methyl iodide formation by analyzing the reaction mixture at 100 °C using different volumes of HI and amount of LiI. Each experiment used 20 mL of absolute methanol, and the reaction mixtures was analyzed after 2, 4, and 6 h.

Table 3. Synthesis of MeI at 100 ΔC under various conditions.

compound	HI	CH3I	MeOAc	MeOH	CH3CO2H	H2O
Run 4: The solution contained 20 mL of HI solution, 20 mL of absolute methanol, and 1.00g of LiI(s).						
Percent at 2 h	16.6	8.8	15.3	26.2	2.0	29.0
Percent at 4 h	16.00	9.0	14.2	26.0	2.2	31.5
Percent at 6 h	15.0	9.1	14.0	25.0	2.3	32.3
Run 5: The solution contained 30 mL of HI solution, 20 mL of absolute methanol, and 1.00 g LiI(s).						
2 h	26.6	1.6	14.8	11.9	6.7	30.2
4h	23.7	2.0	17.2	13.9	3.2	32.2
6h	22.7	2.2	12.7	11.6	2.7	32.0
Run 6: The solution contained 20 mL of HI solution, 20 mL of absolute methanol, and 2.00 g LiI(s).						
2h	24.6	7.1	14.0	22.0	2.2	30.0
4h	20.3	8.3	15.5	23.0	2.4	30.2
6h	20.1	8.7	16.0	21.2	2.3	31.5
Run 7: The solution contained 20 mL of HI solution and 20 mL of absolute methanol without LiI(s).						
2h	26.6	6.5	11.8	23.5	2.2	29.0
4h	23.2	7.0	12.2	25.0	2.2	30.2
6h	20.7	7.3	12.8	25.3	2.6	30.4

Source: Research Findings

The data reported in Table 3 present the results of MeI synthesis at 100°C under four different conditions. These data show that the reaction proceeds more effectively at higher iodide concentrations, but reaction progress is strongly dependent on the balance between the initial HI concentration, LiI addition, and reaction time. Based on the results reported in this table, Run 4 gave the highest CH_3I concentration, increasing from 8.8% at 2 h to 9.1% at 6 h. In this run, 20 mL of HI solution, 20 mL of methanol, and 1.00 g LiI were mixed, suggesting that a smaller HI volume combined with LiI creates a favorable environment for MeI formation. The relatively low HI volume and the presence of added iodide likely promote the S_N2 reaction to produce methyl iodide. At the same time, water increased from 29.0% to 32.3%, indicating that the reaction progresses while the aqueous phase becomes more prominent.

In contrast, Runs 5 and 6 produced lower amounts of CH_3I than Run 4, even though larger volume of HI and a greater amount of LiI were used (30 mL HI in Run 5 and 2.00 g of LiI in Run 6). A comparation of the data reveals that Run 4 consistently yielded a higher concentration of MeI % than Run 7 across all measured time points. At 2 h, the MeI concentration reached 8.8% in Run 4 compared to 6.5% in Run 7. This trend of higher MeI accumulation persisted at at 4 h (9.0 % *vs.* 7.0 %) and 6 h (9.1 % vs. 7.3 %). Because the addition of LiI in Run 4 was the sole difference between the two reaction conditions, these results indicate that LiI plays a beneficial role in promoting MeI formation.

Based on the experimental data presented in the tables, kinetic equations (Eqs. 1and 2) were developed. The resulting reaction rates and kinetic constants (k) for all runs are summarized in Table 4.

$$\frac{d[CH_3I]}{dt} = k_1\,[MeOH][HI] - K_{-1}\,[MeOH][H_2O] \qquad \text{Eq. 1}$$

$$\frac{d[MeOAc]}{dt} = k_2\,[MeOH][CH_3CO_2H] - K_{-2}\,[MeOAc][H_2O] \qquad \text{Eq.2}$$

Table 4. Reaction rates and rate constants for Runs 1–7.

Run	Rate avg % . h-1	K %-1. h-1	Rate avg % . h-1	K %-1. h-1
	MeI		MeOAc	
1	0.25	5.17×10-4	0.13	2.34×10-3
2	0.38	1.03×10-3	0.58	9.04×10-3
3	0.15	4.21×10-4	0.13	1.61×10-3
4	0.08	1.72×10-4	-0.33	-6.02×10-3
5	0.15	4.73×10-4	-0.53	-6.58×10-3
6	0.4	7.40×10-4	0.50	1.03×10-2
7	0.2	3.20×10-4	0.25	4.8×10-3

Source: Research Findings

According to the data reported in Table 4, the average reaction rate for MeI ranged from 0.08 %·h⁻¹ in Run 4 to 0.40 %·h⁻¹ in Run 6, while the kinetic constant varied from 1.72×10^{-4} %⁻¹·h⁻¹ in Run 4 to 1.03×10^{-3} %⁻¹·h⁻¹ in Run 2. These results indicate that the MeI formation rate was generally modest, with Run 6 showing highest apparent reaction rate among the tested conditions. For MeOAc, the highest positive average reaction rate and kinetic constant were also observed in Run 6, with values of 0.50 %·h⁻¹ and 1.03×10^{-2} %⁻¹·h⁻¹, respectively.

In contrast, Runs 4 and 5 showed negative values for both parameters, suggesting an unfavorable or declining trend under those conditions. Overall, the data in Table 4 show that the kinetic performance varied considerably among the runs, and Run 6 exhibited the most favorable apparent kinetic behavior for both products. Based on the data presented in the tables, the kinetic curves of synthesis of MeI and MeOAc are illustrated in Figure 3.

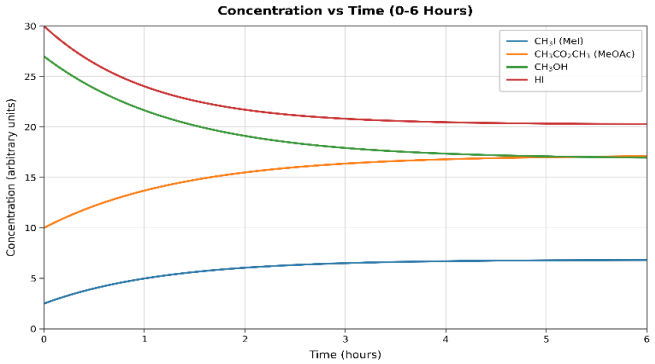


Figure 3. Kinetic curve of synthesis of MeI and MeOAc.

Source: Research Findings

To provide a theoretical foundation for the experimental observations, the interactions between methanol (acting as the nucleophile) and various electrophilic species including H^+, Li^+, LiI, and HI were evaluated using frontier molecular orbital (FMO) theory and computed interaction energies. The results of these theoretical calculations are summarized in Tables 5 and 6.

Table 5. Calculated the ΔE of electron transfer from nucleophile to electrophiles.

compound	Nucleophile (Nu)	Electrophile (E+)			
	MeOH	Li+	H+	HI	LiI
HOMO	-0.263	-2.35	-	-0.283	-0.223
LUMO	+0.067	-0.25	-	-0.035	-0.075
ΔE	-	0.013	0.263	0.228	0.188
		ΔE= ELE+ - EH Nu			

Source: Research Findings

Table 6. Calculated the energy interaction of various compounds.

Compound	CH3OH-H+	CH3OH-Li+	CH3OH-LiI	CH3OH-HI
E (a.u)	-115.65	-123.01	-134.71	-127.67

Source: Research Findings

The result reported in Tables 5 and 6 demonstrate that the synthesis of methyl iodide from methanol is strongly influenced by the presence of HI and LiI, which facilitate both electron transfer and reactant interaction. The calculate electron-transfer energy (ΔE) between methanol (the nucleophile) and the electrophilic species indicates that Li^+ provides the lowest ΔE value, suggesting the most favorable interaction for activation of methanol (Table 5). Furthermore, the data in Table 6 show that the interaction energies of methanol with LiI (covalent form) and HI (covalent bond) are more stabilized than with

H^+ or Li^+ (ion forms), indicating that these species promote the formation of a more reactive complex. Overall, the results suggest that LiI enhances the rate of CH_3I formation by lowering the energetic barrier and stabilizing the reaction pathway, which is consistent with its catalytic role in the Monsanto-type iodination process (Figure 4).

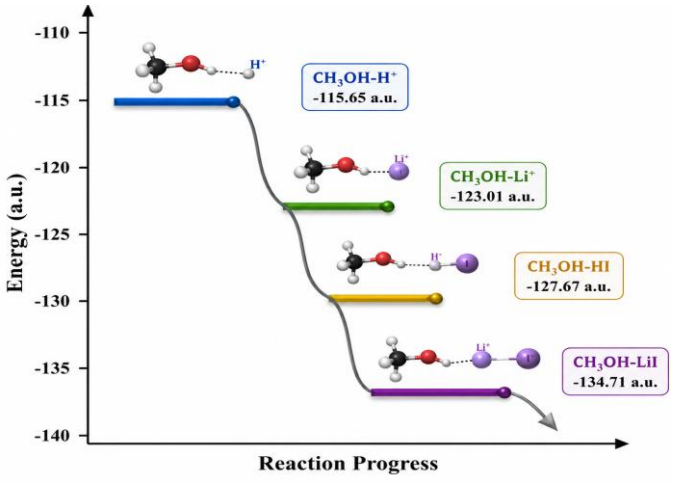


Figure 4. Diagram energy of reaction progress in synthesis of MeI.
Source: Research Findings

4. Conclusions

The present study demonstrates that lithium iodide can effectively promote the conversion of methanol to methyl iodide analogous to certain aspects of Monsanto-type chemistry. Systematic variation of temperature, HI volume, LiI loading, and reaction time revealed that both product distribution and reaction kinetics are strongly dependent on these parameters. Among the temperatures examined, 100 °C was identified as the optimum condition, at which methyl iodide formation is maximized while maintaining operational convenience. The results of this study suggest that methanol iodination proceeds via an S_N2 mechanism. At 100 °C, the combined effects of HI volume and LiI loading were found to be critical. The most favorable composition was obtained using 20 mL of HI, 20 mL methanol, and 1.00 g LiI, which afforded 9.1% CH_3I after 6 h. Increasing the HI volume from 20 mL to 30 mL significantly suppressed CH_3I formation, and although increasing LiI to 2.00 g enhanced the reaction rate, it did not surpass the CH_3I content achieved with 1.00 g LiI. Comparison with the LiI-free system confirmed the promotional role of LiI, leading to higher CH_3I levels at all reaction times. Density functional theory and frontier molecular orbital analyses supported these experimental observations by indicating favorable electronic interactions and stabilizing effects for methanol in the presence of LiI and HI. Overall, the combined experimental and theoretical results establish LiI as an effective promoter for methyl iodide formation and provide insight into optimizing Monsanto-type iodination chemistry through controlled acid and promoter loadings.

Author Contributions

All authors contributed equally to the conception, preparation, and writing of this manuscript.

Conflict of Interest

The authors, while observing publication ethics in the referencing, declare the absence of interest of conflict.

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